

10766712

11/12/06

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NEWS 3 AUG 09 INSPEC enhanced with 1898-1968 archive  
NEWS 4 AUG 28 ADISCTI Reloaded and Enhanced  
NEWS 5 AUG 30 CA(SM)/Caplus(SM) Austrian patent law changes  
NEWS 6 SEP 11 CA/Caplus enhanced with more pre-1907 records  
NEWS 7 SEP 21 CA/Caplus fields enhanced with simultaneous left and right  
truncation  
NEWS 8 SEP 25 CA(SM)/Caplus(SM) display of CA Lexicon enhanced  
NEWS 9 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates  
NEWS 10 SEP 25 CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine  
NEWS 11 SEP 28 CEABA-VTB classification code fields reloaded with new  
classification scheme  
NEWS 12 OCT 19 LOGOFF HOLD duration extended to 120 minutes  
NEWS 13 OCT 19 E-mail format enhanced  
NEWS 14 OCT 23 Option to turn off MARPAT highlighting enhancements available  
NEWS 15 OCT 23 CAS Registry Number crossover limit increased to 300,000 in  
multiple databases  
NEWS 16 OCT 23 The Derwent World Patents Index suite of databases on STN  
has been enhanced and reloaded  
NEWS 17 OCT 30 CHEMLIST enhanced with new search and display field  
NEWS 18 NOV 03 JAPIO enhanced with IPC 8 features and functionality  
NEWS 19 NOV 10 CA/Caplus F-Term thesaurus enhanced  
NEWS 20 NOV 10 STN Express with Discover! free maintenance release Version  
8.01c now available

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT  
MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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NEWS LOGIN Welcome Banner and News Items  
NEWS IPC8 For general information regarding STN implementation of IPC 8  
NEWS X25 X.25 communication option no longer available

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 20:15:59 ON 12 NOV 2006

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 20:16:08 ON 12 NOV 2006

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STRUCTURE FILE UPDATES: 10 NOV 2006 HIGHEST RN 913001-11-3

DICTIONARY FILE UPDATES: 10 NOV 2006 HIGHEST RN 913001-11-3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

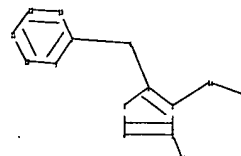
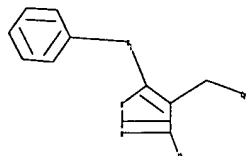
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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Uploading C:\Program Files\Stnexp\Queries\1076671212.str



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chain nodes :
6 14 15 16
ring nodes :
1 2 3 4 5 7 9 10 11 12 13
chain bonds :
1-6 2-14 3-16 6-7 14-15
ring bonds :
1-2 1-5 2-3 3-4 4-5 7-9 7-13 9-10 10-11 11-12 12-13
exact/norm bonds :
1-5 1-6 3-4 3-16 4-5 6-7 14-15
exact bonds :
1-2 2-3 2-14
normalized bonds :
7-9 7-13 9-10 10-11 11-12 12-13
isolated ring systems :
containing 1 : 7 :

```

G1:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:CLASS 15:Atom 16:CLASS

10766712.

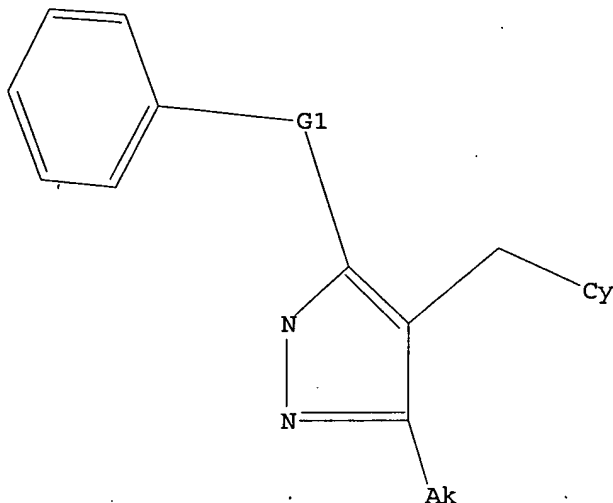
11/12/06

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 20:16:27 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 259 TO ITERATE

100.0% PROCESSED 259 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 4215 TO 6145

PROJECTED ANSWERS: 5 TO 234

L2 5 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 20:16:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 5016 TO ITERATE

100.0% PROCESSED 5016 ITERATIONS

144 ANSWERS

SEARCH TIME: 00.00.01

L3 144 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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167.15

FILE 'CAPLUS' ENTERED AT 20:16:38 ON 12 NOV 2006

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FILE COVERS 1907 - 12 Nov 2006 VOL 145 ISS 21  
FILE LAST UPDATED: 10 Nov 2006 (20061110/ED)

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<http://www.cas.org/infopolicy.html>

=> s l3

L4 30 L3

=> s l4 and HIV

68922 HIV

96 HIVS

68938 HIV

(HIV OR HIVS)

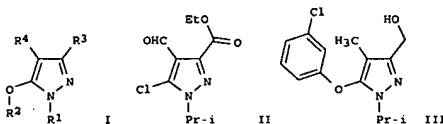
L5 3 L4 AND HIV

=> D IBIB ABS HITSTR TOT

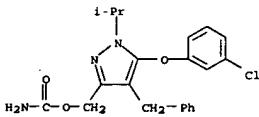
L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2004:718518 CAPLUS  
DOCUMENT NUMBER: 141:243549  
TITLE: Preparation of pyrazole derivatives as non-nucleoside  
reverse transcriptase inhibitors for the treatment of  
HIV disorders and compositions thereof  
INVENTOR(S): Dunn, James Patrick; Hogg, Joan Heather; Mirzadegan,  
Taraneh; Swallow, Steven  
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.  
SOURCE: PCT Int. Appl., 90 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

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WO 2004074257	A1	200404902	WO 2004-EP1477	200402017
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AU 2004213134	A1	20040902	AU 2004-213134	200402017
CA 2515151	AA	20040902	CA 2004-2515151	200402017
EP 1597235	A1	20051117	EP 200511607	200402017
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
BR 2004007591	A	20060214	BR 2004-7591	200402017
CN 1751028	A	20060322	CN 2004-80004406	200402017
JP 2006515339	T2	20060525	JP 2006-500034	200402017
US 2004192666	A1	20040930	US 2004-781373	200402018
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			WO 2004-EP14774	A 200402017

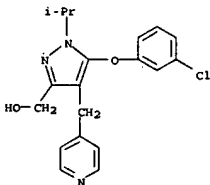
OTHER SOURCE(S) : MARPAT 141:243549  
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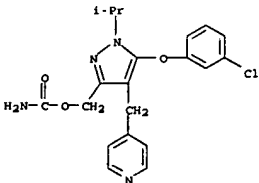
L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 750637-01-5 CAPLUS  
CN 1H-Pyrazole-3-methanol, 5-(3-chlorophenoxy)-1-(1-methylethyl)-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



RN 750637-02-6 CAPLUS  
CN 1H-Pyrazole-3-methanol, 5-(3-chlorophenoxy)-1-(1-methylethyl)-4-(4-pyridinylmethyl)-, carbamate (ester) (9CI) (CA INDEX NAME)



RN 750637-45-7 CAPLUS  
CN 1H-Pyrazole-3-ethanol, 5-(3,5-dichlorophenoxy)-1-ethyl-4-(phenylmethyl)-  
(9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

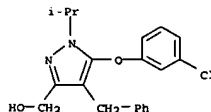
AB This invention relates to novel pyrazole derivs. of formula I [wherein R1 is (halo/cyclo/alkoxy)alkyl, alk(en/yn)yl, or substituted Ph/benzyl; R2 is (un)substituted Ph or pyridyl; R3 is substituted (alkoxy/cyclo)alkyl, (un)substituted alk(en/alkoxy)amino, C=O/Y or -X(C=O/Y, etc.; X and Y independently are O or (un)substituted NH; Z is H, OH, alkoxy, (un)substituted amino or (alkoxy)alkyl; R4 is (un)substituted alk(en/yn)yl, cyclo/alkoxyalkyl], pharmaceutically acceptable salts and esters thereof, methods to inhibit or modulate human immunodeficiency virus (HIV) reverse transcriptase with I, and pharmaceutical compns. of I admixed with at least one solvent, carrier or excipient.

The compds. are useful for treating disorders in which HIV and genetically related viruses are implicated, such as HIV infection, AIDS or ARC. Thus, pyrazole II (preparation given) was etherified with 3-chlorophenol, followed by selective reduction with NaBH4 to give an alc., which was then converted to its iodide with diphosphorus tetraiodide, and finally reduced with LAH to afford III. The compds. showed activity in the HIV-1 RT assay and in an anti-HIV antiviral assay with IC50 of 0.5-1000 nM and 0.5-5000 nM, resp.

IT 7506362-99-8P 750637-00-4P 750637-01-5P 750637-02-6P 750637-45-7P 750637-46-8P  
RI PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

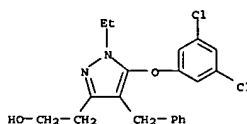
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reverse (uses)
reverse (drug candidate; preparation of pyrazole derivs. as non-nucleoside
reverse transcriptase inhibitors)
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RN 750636-99-8 CAPLUS  
CN 1H-Pyrazole-3-methanol, 5-(3-chlorophenoxy)-1-(1-methylethyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

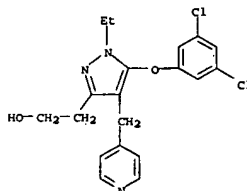


RN 750637-00-4 CAPLUS  
CN 1H-Pyrazole-3-methanol, 5-(3-chlorophenoxy)-1-(1-methylethyl)-4-(phenylmethyl)-, carbamate (ester) (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 750637-46-8 CAPLUS  
CN 1H-Pyrazole-3-ethanol, 5-(3,5-dichlorophenoxy)-1-ethyl-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE  
FORMAT

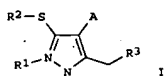
10766712

11/12/06

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN  
 ACCESSION NUMBER: 2002:964349 CAPLUS  
 DOCUMENT NUMBER: 138:39280  
 TITLE: Preparation of pyrazoles as HIV reverse transcriptase inhibitors  
 INVENTOR(S): Dymock, Brian William; Gill, Adrian Liam; Jones, Philip Stephen; Parkes, Kevin Edward Burdon; Parratt, Martin John  
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.  
 SOURCE: PCT Int. Appl., 64 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

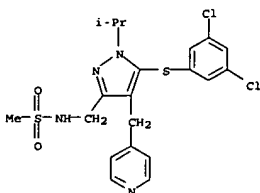
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WO 2002100853	A1	20021219	WO 2002-EP5898	20020529
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RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CH, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 6538015	B1	20030325	US 2002-154585	20020524
CA 2448058	AA	20021219	CA 2002-2448058	20020529
EP 1401826	A1	20040331	EP 2002-758207	20020529
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2002010158	A	20040608	BR 2002-10158	20020529
CN 1527829	A	20040908	CN 2002-811197	20020529
JP 2004532276	T2	20041021	JP 2003-503620	20020529
ZA 2003008781	A	20050211	ZA 2003-8781	20031111
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			WO 2002-EP5898	W 20020529

OTHER SOURCE(S): MARPAT 138:39280  
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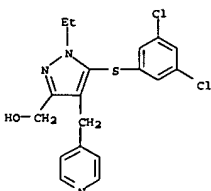


AB The title compds. [I: R1 = (un)substituted alkyl; R2 = (un)substituted aryl; R3 = OH, NH2, N3, OH, etc.; A = (un)substituted alkyl, arylmethyl, heterocyclylmethyl, etc.] which are inhibitors of the human

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)  
 RN 478620-57-4 CAPLUS  
 CN Methanesulfonamide, N-[(5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-1H-pyrazol-3-yl)methyl]- (9CI) (CA INDEX NAME)

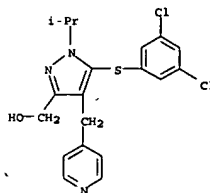


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 478620-44-9P 478620-45-0P 478620-46-1P  
 478620-47-2P 478620-48-3P 478620-49-4P  
 478620-50-7P 478620-52-9P 478620-53-0P  
 478620-54-1P 478620-56-3P 478620-58-5P  
 478620-68-7P 478620-72-3P 478620-73-4P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyrazoles as HIV reverse transcriptase inhibitors)  
 RN 478620-41-6 CAPLUS  
 CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-1-ethyl-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

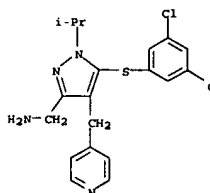


RN 478620-42-7 CAPLUS  
 CN 1H-Pyrazole-3-methanol, 5-[(3,5-difluorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)  
 immunodeficiency virus reverse transcriptase enzyme which is involved in viral replication, and consequently may be used as therapeutic agents for HIV mediated process, were prepd. E.g., a 9-step synthesis of 1 [R1 = iso-Pr; R2 = 3,5-Cl2C6H3; R3 = OH; A = (4-pyridyl)methyl], starting with tert-Bu carbazate and acetone, was given. The compds. I range in IC50 activity from about 0.5 to about 5000 nM in the anti-HIV assay.  
 IT 478620-40-5P 478620-55-2P 478620-57-4P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of pyrazoles as HIV reverse transcriptase inhibitors)  
 RN 478620-40-5 CAPLUS  
 CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

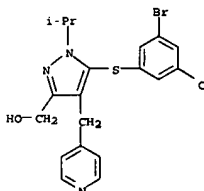


RN 478620-55-2 CAPLUS  
 CN 1H-Pyrazole-3-methanamine, 5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

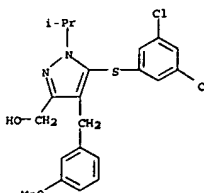


L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS ON STN (Continued)

RN 478620-43-8 CAPLUS  
 CN 1H-Pyrazole-3-methanol, 5-[(3-bromo-5-chlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



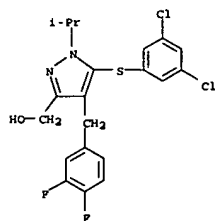
RN 478620-44-9 CAPLUS  
 CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-4-[(3-methoxyphenyl)methyl]-1-(1-methylethyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

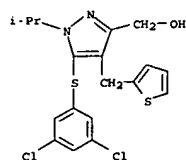
RN 478620-45-0 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-4-[(3,4-difluorophenyl)methyl]-1-(1-methylethyl)- (9CI) (CA INDEX NAME)



RN 478620-46-1 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(2-thienylmethyl)- (9CI) (CA INDEX NAME)



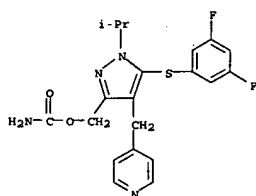
RN 478620-47-2 CAPLUS

CN 1H-Pyrazole-3-methanol, 4-[(5-bromo-2-methyl-4-pyrimidinyl)methyl]-5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

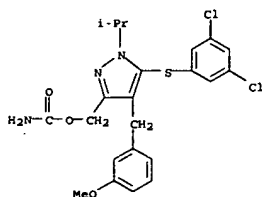
RN 478620-50-7 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[(3,5-difluorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-, carbamate (ester) (9CI) (CA INDEX NAME)



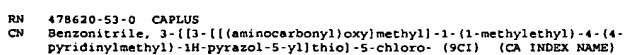
RN 478620-52-9 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-4-[(3-methoxyphenyl)methyl]-1-(1-methylethyl)-, carbamate (ester) (9CI) (CA INDEX NAME)

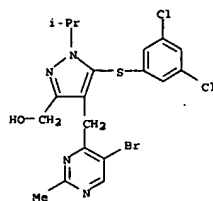


RN 478620-53-0 CAPLUS

CN Benzonitrile, 3-[[3-[(aminocarbonyl)oxy]methyl]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-1H-pyrazol-5-yl]thio]-5-chloro- (9CI) (CA INDEX NAME)

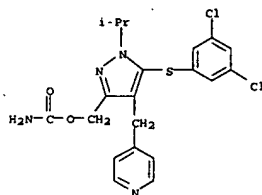


L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



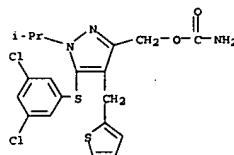
RN 478620-48-3 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-, carbamate (ester) (9CI) (CA INDEX NAME)

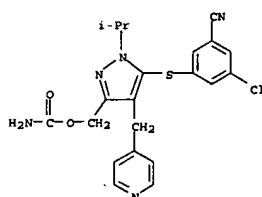


RN 478620-49-4 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(2-thienylmethyl)-, carbamate (ester) (9CI) (CA INDEX NAME)

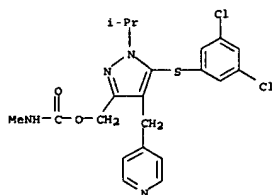


L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



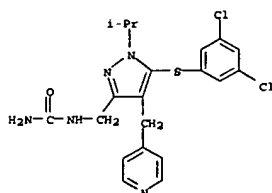
RN 478620-54-1 CAPLUS

CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-, methylcarbamate (ester) (9CI) (CA INDEX NAME)



RN 478620-56-3 CAPLUS

CN Urea, [[5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-1H-pyrazol-3-yl]methyl]- (9CI) (CA INDEX NAME)

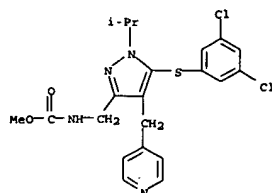




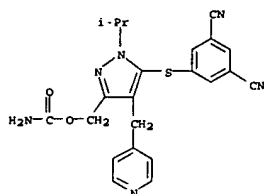
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11/12/06

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 RN 478620-58-5 CAPLUS  
 CN Carbamic acid, [[5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-1H-pyrazol-3-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

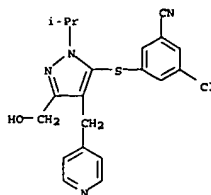


RN 478620-68-7 CAPLUS  
 CN 1,3-Benzenedicarbonitrile, 5-[[3-[[[(aminocarbonyl)oxy]methyl]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-1H-pyrazol-5-yl]thio]- (9CI) (CA INDEX NAME)

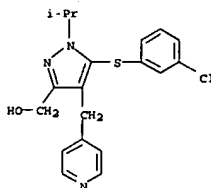


RN 478620-72-3 CAPLUS  
 CN Benzonitrile, 3-chloro-5-[[3-(hydroxymethyl)-1-(1-methylethyl)-4-(4-pyridinylmethyl)-1H-pyrazol-5-yl]thio]- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



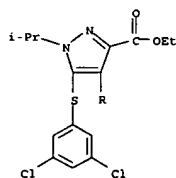
RN 478620-73-4 CAPLUS  
 CN 1H-Pyrazole-3-methanol, 5-[(3-chlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



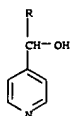
IT 478620-63-2P 478620-64-3P 478620-65-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pyrazoles as HIV reverse transcriptase inhibitors)  
 RN 478620-63-2 CAPLUS  
 CN 1H-Pyrazole-3-carboxylic acid, 5-[(3,5-dichlorophenyl)thio]-4-(hydroxy-4-pyridinylmethyl)-1-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

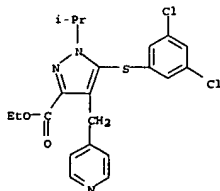
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PAGE 2-A

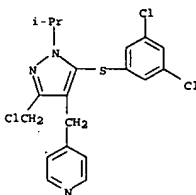


RN 478620-64-3 CAPLUS  
 CN 1H-Pyrazole-3-carboxylic acid, 5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-4-(4-pyridinylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 478620-65-4 CAPLUS  
 CN Pyridine, 4-[(3-(chloromethyl)-5-[(3,5-dichlorophenyl)thio]-1-(1-methylethyl)-1H-pyrazol-4-yl)methyl]-, hydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



•x HCl

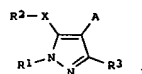
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2002:325538 CAPLUS  
 DOCUMENT NUMBER: 136:325538  
 TITLE: Preparation of pyrazoles for the treatment of viral diseases  
 INVENTOR(S): Dymock, Brian William; Jones, Philip Stephen; Merrett, John Herbert; Parratt, Martin John  
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.  
 SOURCE: PCT Int. Appl., 108 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

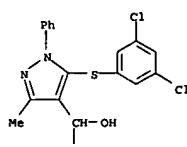
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NO 2002030907	A1	20020418	NO 2001-EP11474	20011004
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CP, CG, CI, CH, CM, GN, GO, GW, ML, MR, NE, SN, TD, TG				
US 2003018197	A1	20030123	US 2001-956656	20010920
US 6698887	B2	20040302		
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AU 2002021651	A5	20020422	AU 2002-21651	20011004
BR 2001014483	A	20030701	BR 2001-14483	20011004
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JP 2004511469	T2	20040415	JP 2002-534293	20011004
NZ 524740	A	20050930	NZ 2001-524740	20011004
CN 1680333	A	20051012	CN 2005-10008832	20011004
RU 2270832	C2	20060227	RU 2003-112610	20011004
ZA 2003002519	A	20040630	ZA 2003-2519	20030331
NO 2003001615	A	20030523	NO 2003-1615	20030409
US 2004192752	A1	20040930	US 2004-766712	20040127
HK 1061021	A1	20050527	HK 2004-103975	20040603
PRIORITY APPLN. INFO.:			GB 2000-24795	A 200001010

OTHER SOURCE(S): MARPAT 136:325538  
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L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

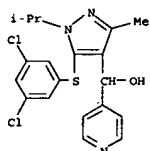


AB The title compds. [I; R1 = alkyl, cycloalkyl, aryl, etc.; R2 = aryl, (un)substituted Ph; R3 = alkyl, alkoxyalkyl; A = CH2(arylalkylamino), CH2(arylalkoxy), etc.; X = S, O] that are inhibitors of the human immunodeficiency virus reverse transcriptase enzyme which is involved in viral replication, were prepared E.g., a 3-step synthesis of pyrazole 1  
 (R1 = Ph; R2 = 3,5-Cl2C6H3; X = S; R3 = Me; A = CH2Ph] which showed IC50 of 2060 nM against HIV-1 reverse transcriptase, was given.  
 IT 412325-70-3P 412326-18-2P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of pyrazoles as inhibitors of the HIV reverse transcriptase)  
 RN 412325-70-3 CAPLUS  
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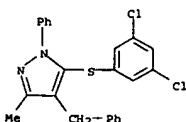


RN 412326-18-2 CAPLUS  
 CN 4-Pyridinemethanol, 5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

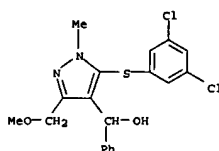


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 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (preparation of pyrazoles as inhibitors of the HIV reverse transcriptase)  
 RN 412325-66-7 CAPLUS  
 CN 1H-Pyrazole, 5-[(3,5-dichlorophenyl)thio]-3-methyl-1-phenyl-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

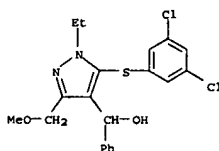


RN 412325-68-9 CAPLUS  
 CN 1H-Pyrazole-4-methanol, 5-[(3,5-dichlorophenyl)thio]-3-(methoxymethyl)-1-methyl-1-phenyl- (9CI) (CA INDEX NAME)

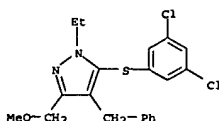
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412325-73-6 CAPLUS  
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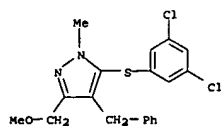


RN 412325-75-8 CAPLUS  
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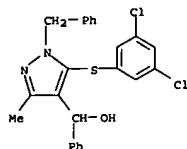


RN 412325-77-0 CAPLUS  
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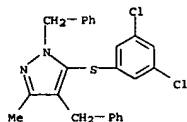
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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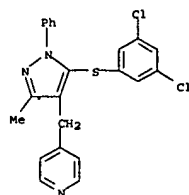


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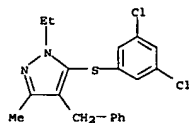


RN 412325-83-8 CAPLUS  
CN Pyridine, 4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-phenyl-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

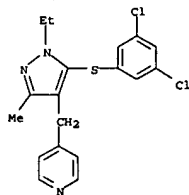
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412325-85-0 CAPLUS  
CN 1H-Pyrazole, 5-[(3,5-dichlorophenyl)thio]-1-ethyl-3-methyl-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

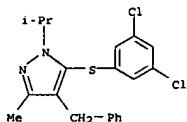


RN 412325-86-1 CAPLUS  
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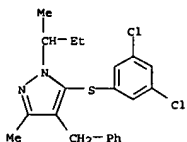


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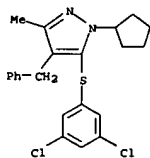
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
CN 1H-Pyrazole, 5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 412326-01-3 CAPLUS  
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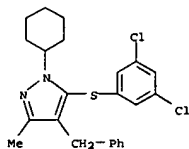


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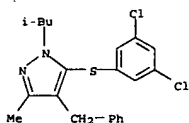


RN 412326-04-6 CAPLUS  
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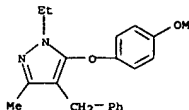
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412326-06-8 CAPLUS  
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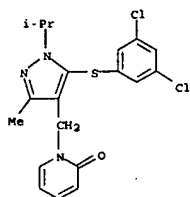


RN 412326-08-0 CAPLUS  
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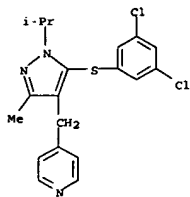


RN 412326-14-8 CAPLUS  
CN 2(1H)-Pyridinone, 1-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

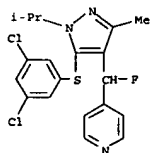
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412326-19-3 CAPLUS  
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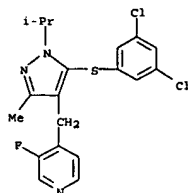


RN 412326-21-7 CAPLUS  
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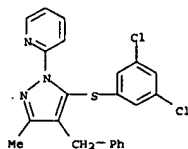


L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

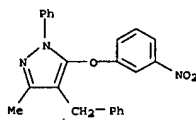
RN 412326-23-9 CAPLUS  
 CN Pyridine, 4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-3-fluoro- (9CI) (CA INDEX NAME)



RN 412326-26-2 CAPLUS  
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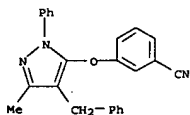


RN 412326-27-3 CAPLUS  
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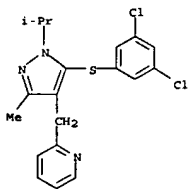


RN 412326-29-5 CAPLUS

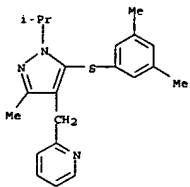
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 CN Benzonitrile,  
 3-[[3-methyl-1-phenyl-4-(phenylmethyl)-1H-pyrazol-5-yl]oxy]- (9CI) (CA INDEX NAME)



RN 412326-31-9 CAPLUS  
 CN Pyridine, 2-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

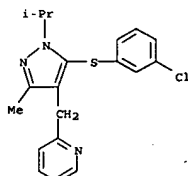


RN 412326-34-2 CAPLUS  
 CN Pyridine, 2-[[5-[(3,5-dimethylphenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

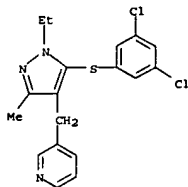


RN 412326-35-3 CAPLUS  
 CN Pyridine, 2-[[5-[(3-chlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

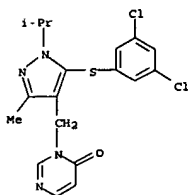
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412326-38-6 CAPLUS  
 CN Pyridine, 3-[[5-[(3,5-dichlorophenyl)thio]-1-ethyl-3-methyl-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

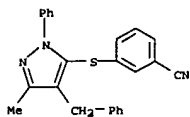


RN 412326-40-0 CAPLUS  
 CN 4(3H)-Pyrimidinone, 3-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

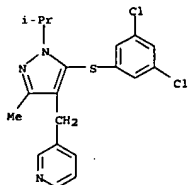


RN 412326-42-3 CAPLUS  
 CN Benzonitrile,  
 3-[[3-methyl-1-phenyl-4-(phenylmethyl)-1H-pyrazol-5-yl]thio]-

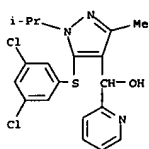
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
(9CI) (CA INDEX NAME)



RN 412326-44-4 CAPLUS  
CN Pyridine, 3-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

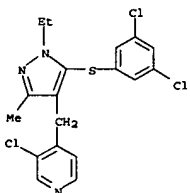


RN 412326-46-6 CAPLUS  
CN 2-Pyridinemethanol, α-[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]- (9CI) (CA INDEX NAME)

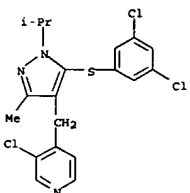


RN 412326-52-4 CAPLUS  
CN Pyrimidine, 4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

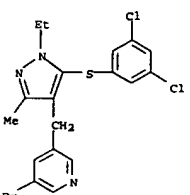
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



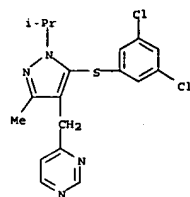
RN 412326-61-5 CAPLUS  
CN Pyridine, 3-chloro-4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)



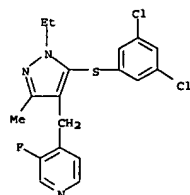
RN 412326-65-9 CAPLUS  
CN Pyridine, 3-bromo-5-[[5-[(3,5-dichlorophenyl)thio]-1-ethyl-3-methyl-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



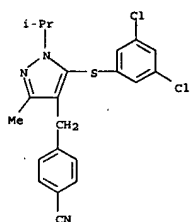
RN 412326-57-9 CAPLUS  
CN Pyridine, 4-[[5-[(3,5-dichlorophenyl)thio]-1-ethyl-3-methyl-1H-pyrazol-4-yl]methyl]-3-fluoro- (9CI) (CA INDEX NAME)



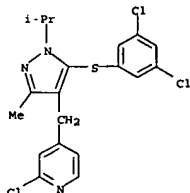
RN 412326-59-1 CAPLUS  
CN Pyridine, 3-chloro-4-[[5-[(3,5-dichlorophenyl)thio]-1-ethyl-3-methyl-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 412326-67-1 CAPLUS  
CN Benzonitrile, 4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

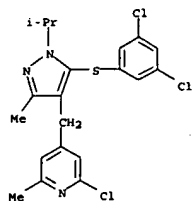


RN 412326-69-3 CAPLUS  
CN Pyridine, 2-chloro-4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

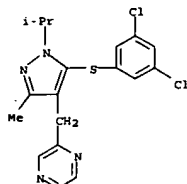


RN 412326-71-7 CAPLUS  
CN Pyridine, 2-chloro-4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-6-methyl- (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

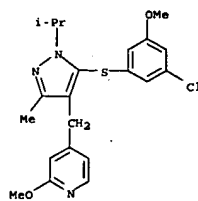


RN 412326-73-9 CAPLUS  
 CN Pyrazine, [[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

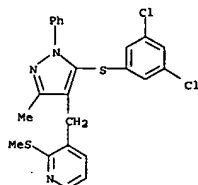


RN 412326-75-1 CAPLUS  
 CN Pyridine, 4-[[5-[(3-chloro-5-methoxyphenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-2-methoxy- (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

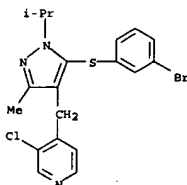


RN 412326-77-3 CAPLUS  
 CN Pyridine, 3-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-phenyl-1H-pyrazol-4-yl]methyl]-2-(methylthio)- (9CI) (CA INDEX NAME)

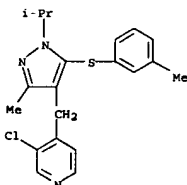


RN 412326-79-5 CAPLUS  
 CN Pyridine, 4-[[5-[(3-bromophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-3-chloro- (9CI) (CA INDEX NAME)

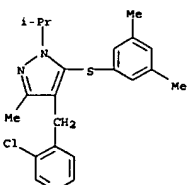
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412326-81-9 CAPLUS  
 CN Pyridine, 3-chloro-4-[[3-methyl-1-(1-methylethyl)-5-[(3-methylphenyl)thio]-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

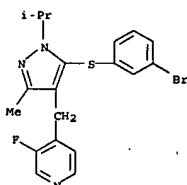


RN 412326-83-1 CAPLUS  
 CN Pyridine, 3-chloro-4-[[5-[(3,5-dimethylphenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

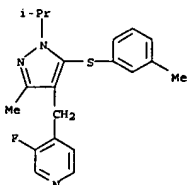


RN 412326-85-3 CAPLUS

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 CN Pyridine, 4-[[5-[(3-bromophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-3-fluoro- (9CI) (CA INDEX NAME)



RN 412326-87-5 CAPLUS  
 CN Pyridine, 3-fluoro-4-[[3-methyl-1-(1-methylethyl)-5-[(3-methylphenyl)thio]-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

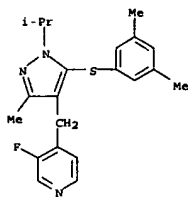


RN 412326-89-7 CAPLUS  
 CN Pyridine, 4-[[5-[(3,5-dimethylphenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-3-fluoro- (9CI) (CA INDEX NAME)

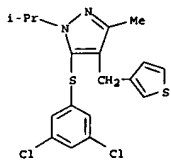
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L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

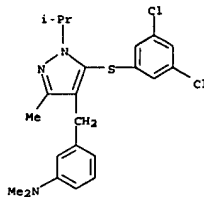


RN 412326-91-1 CAPLUS  
 CN 1H-Pyrazole,  
 5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-4-(3-thienylmethyl)- (9CI) (CA INDEX NAME)

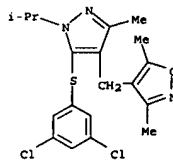


RN 412326-93-3 CAPLUS  
 CN Benzenamine, 3-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

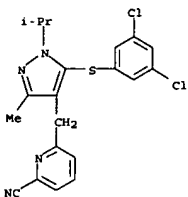


RN 412326-95-5 CAPLUS  
 CN Isoxazole,  
 4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

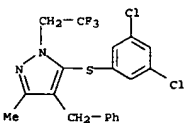


RN 412326-97-7 CAPLUS  
 CN 2-Pyridinecarbonitrile, 6-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)

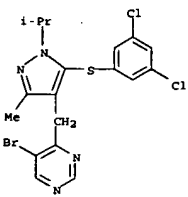
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412327-50-5 CAPLUS  
 CN 1H-Pyrazole, 5-[(3,5-dichlorophenyl)thio]-3-methyl-4-(phenylmethyl)-1-(2,2,2-trifluoroethyl)- (9CI) (CA INDEX NAME)



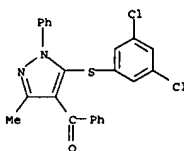
RN 412327-54-9 CAPLUS  
 CN Pyrimidine, 5-bromo-4-[[5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]methyl]- (9CI) (CA INDEX NAME)



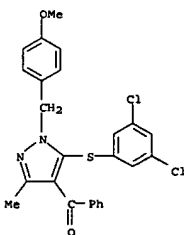
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 412327-18-5P 412327-24-3P 412327-26-5P  
 412327-36-7P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 (prepn. of pyrazoles as inhibitors of the HIV reverse transcriptase)

RN 412327-01-6 CAPLUS  
 CN Methanone, [5-[(3,5-dichlorophenyl)thio]-3-methyl-1-phenyl-1H-pyrazol-4-yl]phenyl- (9CI) (CA INDEX NAME)

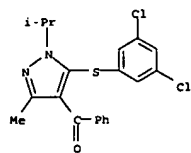


RN 412327-13-0 CAPLUS  
 CN Methanone, [5-[(3,5-dichlorophenyl)thio]-1-[(4-methoxyphenyl)methyl]-3-methyl-1H-pyrazol-4-yl]phenyl- (9CI) (CA INDEX NAME)

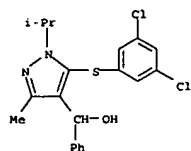


RN 412327-17-4 CAPLUS  
 CN Methanone, [5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-1H-pyrazol-4-yl]phenyl- (9CI) (CA INDEX NAME)

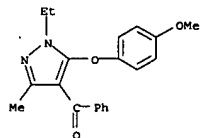
L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412327-18-5 CAPLUS  
 CN 1H-Pyrazole-4-methanol, 5-[(3,5-dichlorophenyl)thio]-3-methyl-1-(1-methylethyl)-α-phenyl- (9CI) (CA INDEX NAME)

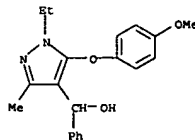


RN 412327-24-3 CAPLUS  
 CN Methanone, [1-ethyl-5-(4-methoxyphenoxy)-3-methyl-1H-pyrazol-4-yl]phenyl- (9CI) (CA INDEX NAME)

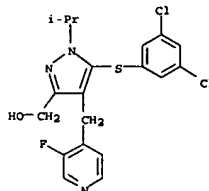


RN 412327-26-5 CAPLUS  
 CN 1H-Pyrazole-4-methanol, 1-ethyl-5-(4-methoxyphenoxy)-3-methyl-α-phenyl- (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 412327-36-7 CAPLUS  
 CN 1H-Pyrazole-3-methanol, 5-[(3,5-dichlorophenyl)thio]-4-[(3-fluoro-4-pyridinyl)methyl]-1-(1-methylethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE  
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LOGOFF? (Y)/N/HOLD:Y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

19.58

186.73

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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